

SeRC Electronic Structure Community

Kick-off

April 7-8 2011, Engsholm Slott, Mörkö

Thursday 7/4

12.00 Lunch

Session 1 Chair: Hans Ågren

13.00-13.20 *Welcome and General Presentation of SeRC Electronic Structure*
Anna Delin (SeRC ES community coordinator, KTH)

13.20-14.10 *Keynote talk: Quantum chemistry: wave-function and density-functional methods*
Trygve Helgaker, Oslo Universitet

14.10-14.50 *eSENCE e-Science Center*
Kersti Hermansson, Uppsala University

14.50-15.20 Coffee + check-in

Session 2 Chair: Kersti Hermansson

15.20-16.00 *Chalmers e-Science Center*
Per Hyldgaard, Chalmers

16.00-16.40 *Electronic structure research at Linneaus University*
Carlo Canali and Magnus Paulsson, Linneaus University

16.40-17.00 Break

17.00-17.40 *SeRC at Linköping University*
Igor Abrikosov, Linköping University

Session 3 Chair: Anna Delin

17.40-18.45 *Panel discussion*

19.00 Dinner

Friday 8/4

07.30 Breakfast + check-out

Session 4 Chair: Anatoly Belonoshko

08.30-09.00 *Application Experts and the Application Knowledge Base*
Torben Rasmussen, NSC

09.00-09.30	<i>PRACE - The kernel of application experts and HPC systems in EU</i> Lilit Axner, PDC
09.30-10.00	<i>Challenges in time-dependent DFT</i> Zilvinas Rinkevicius, KTH
10.00-10.30	Coffee + poster session
<i>Session 5</i>	<i>Chair: Igor Abrikosov</i>
10.30-11.00	<i>New developments in dynamical mean-field theory</i> Leonid Pourovskii, Linköping University and École Polytechnique, Paris
11.00-11.30	<i>Spin dynamics from first principles</i> Lars Bergqvist, KTH
11.30-12.00	<i>Interface electronic effects in bulk-heterojunction systems</i> Mathieu Linares, Linköping University
12.15	Lunch

